

Cyclophosphamide
50-18-0 | DTXSID5020364

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 251 °C

Global applicability domain: Outside

Local applicability domain index: 2.13e-01

Confidence level: 4.54e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-Butylbenzenesulfonamide

Measured: 314

Predicted: 286

[Image not found](#)

Ethyl benzylcarbamate

Measured: 230

Predicted: 255

[Image not found](#)

1,3-Propanediamine, N,N-dibutyl-

Measured: 205

Predicted: 205

[Image not found](#)

1,4-Piperazinedicarboxylic acid, diethyl ester

Measured: 315

Predicted: 304

[Image not found](#)

Etridiazole

Measured: 188

Predicted: 231